



Full wwPDB X-ray Structure Validation Report i

Feb 28, 2014 – 02:35 PM GMT

PDB ID : 2YFQ
Title : Crystal structure of Glutamate dehydrogenase from Peptoniphilus asaccharolyticus
Authors : Oliveira, T.; Panjikar, S.; Carrigan, J.B.; Sharkey, M.A.; Hamza, M.; Engel, P.C.; Khan, A.R.
Deposited on : 2011-04-07
Resolution : 2.94 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

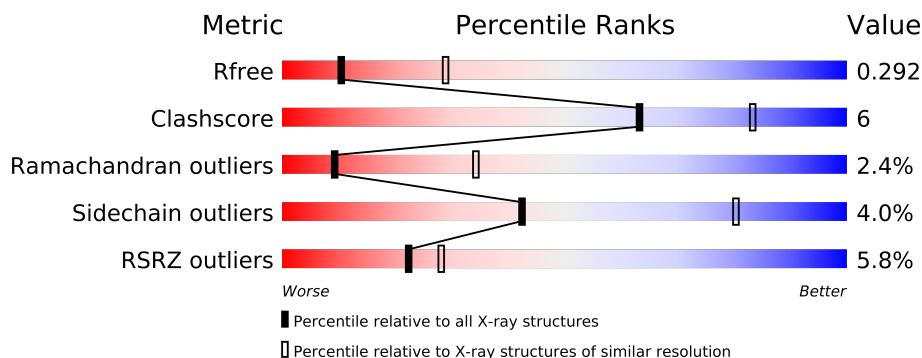
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.94 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	66092	1424 (2.98-2.90)
Clashscore	79885	1761 (2.98-2.90)
Ramachandran outliers	78287	1708 (2.98-2.90)
Sidechain outliers	78261	1710 (2.98-2.90)
RSRZ outliers	66119	1425 (2.98-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	421	
1	B	421	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	SO4	A	1422	-	X

2 Entry composition i

There are 3 unique types of molecules in this entry. The entry contains 6108 atoms, of which 0 are hydrogen and 0 are deuterium.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called NAD-SPECIFIC GLUTAMATE DEHYDROGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	395	Total	C	N	O	S	0	0	0
			3033	1925	516	577	15			
1	B	397	Total	C	N	O	S	0	0	0
			3049	1935	518	581	15			

- Molecule 2 is SULFATE ION (three-letter code: SO₄) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is water.

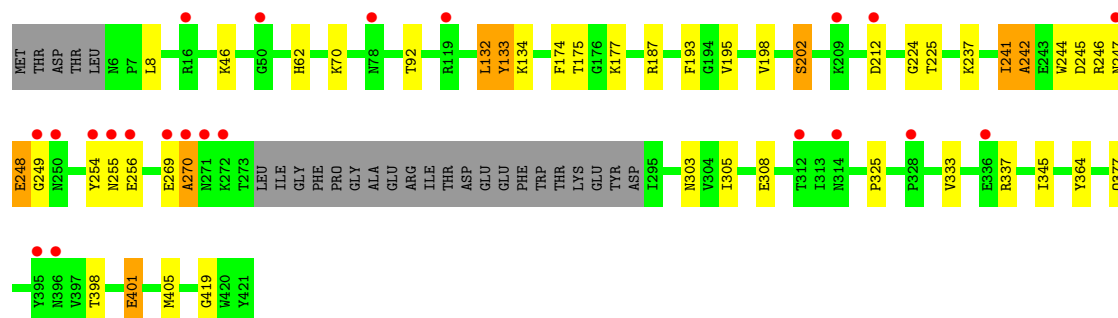
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	4	Total 4	O 4	0	0
3	B	2	Total 2	O 2	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

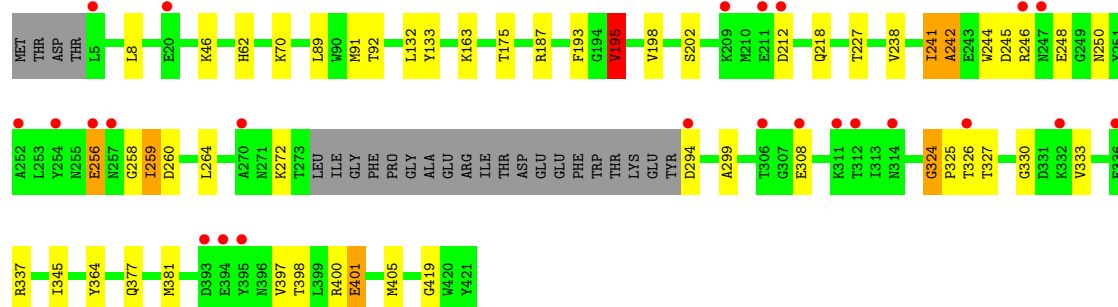
• Molecule 1: NAD-SPECIFIC GLUTAMATE DEHYDROGENASE

Chain A: 



• Molecule 1: NAD-SPECIFIC GLUTAMATE DEHYDROGENASE

Chain B: 



4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	153.31Å 153.31Å 318.99Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.94 19.74 – 2.94	Depositor EDS
% Data completeness (in resolution range)	97.8 (20.00-2.94) 91.1 (19.74-2.94)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.59 (at 2.93Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.242 , 0.287 0.256 , 0.292	Depositor DCC
R_{free} test set	935 reflections (3.44%)	DCC
Wilson B-factor (Å ²)	63.6	Xtriage
Anisotropy	0.002	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 44.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	3 of 28077 reflections (0.011%)	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	6108	wwPDB-VP
Average B, all atoms (Å ²)	79.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 70.89 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 2.8888e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.63	5/3092 (0.2%)	0.70	1/4183 (0.0%)
1	B	0.63	6/3108 (0.2%)	0.69	1/4205 (0.0%)
All	All	0.63	11/6200 (0.2%)	0.70	2/8388 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	2
All	All	0	3

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	133	TYR	CE2-CZ	-7.69	1.28	1.38
1	A	133	TYR	CE1-CZ	-7.09	1.29	1.38
1	B	195	VAL	CB-CG1	-6.83	1.38	1.52
1	A	195	VAL	CB-CG2	-6.78	1.38	1.52
1	A	133	TYR	CE2-CZ	-6.47	1.30	1.38
1	B	133	TYR	CG-CD1	-6.01	1.31	1.39
1	B	195	VAL	CB-CG2	-5.84	1.40	1.52
1	B	133	TYR	CE1-CZ	-5.83	1.30	1.38
1	A	133	TYR	CG-CD1	-5.72	1.31	1.39
1	B	133	TYR	CG-CD2	-5.71	1.31	1.39
1	A	133	TYR	CG-CD2	-5.63	1.31	1.39

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	246	ARG	N-CA-C	5.11	124.80	111.00
1	B	246	ARG	N-CA-C	5.11	124.80	111.00

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	255	ASN	Peptide
1	B	294	ASP	Peptide
1	B	324	GLY	Peptide

5.2 Close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3033	0	21	17	0
1	B	3049	0	21	19	0
2	A	10	0	0	1	0
2	B	10	0	0	2	0
3	A	4	0	0	0	0
3	B	2	0	0	0	0
All	All	6108	0	42	34	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 6.

All (34) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:187:ARG:NH1	2:B:1422:SO4:O1	2.00	0.94
1:A:187:ARG:NH1	2:A:1423:SO4:O2	2.21	0.74
1:B:327:THR:O	1:B:330:GLY:N	2.27	0.66
1:A:198:VAL:O	1:A:202:SER:OG	2.19	0.60
1:B:198:VAL:O	1:B:202:SER:OG	2.23	0.57
1:A:70:LYS:NZ	1:A:175:THR:OG1	2.37	0.56
1:A:419:GLY:O	1:B:46:LYS:NZ	2.39	0.54
1:B:70:LYS:NZ	1:B:175:THR:OG1	2.40	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:62:HIS:CD2	1:B:92:THR:OG1	2.61	0.53
1:A:241:ILE:O	1:A:242:ALA:CB	2.57	0.53
1:B:195:VAL:CG1	1:B:227:THR:CG2	2.87	0.53
1:B:241:ILE:O	1:B:242:ALA:CB	2.57	0.52
1:B:326:THR:OG1	1:B:400:ARG:NH2	2.42	0.52
1:A:244:TRP:CE2	1:A:245:ASP:O	2.65	0.49
1:B:401:GLU:O	1:B:405:MET:SD	2.71	0.49
1:B:238:VAL:O	1:B:258:GLY:O	2.31	0.48
1:A:193:PHE:CD1	1:A:377:GLN:NE2	2.81	0.48
1:B:244:TRP:CE2	1:B:245:ASP:O	2.66	0.48
1:A:269:GLU:O	1:A:270:ALA:CB	2.62	0.47
1:A:46:LYS:NZ	1:B:419:GLY:O	2.48	0.46
1:B:193:PHE:CD1	1:B:377:GLN:NE2	2.84	0.46
1:A:132:LEU:O	1:A:134:LYS:N	2.49	0.46
1:B:91:MET:CE	2:B:1423:SO4:O1	2.65	0.45
1:A:132:LEU:O	1:A:133:TYR:C	2.55	0.45
1:A:174:PHE:O	1:A:177:LYS:NZ	2.50	0.44
1:A:247:ASN:O	1:A:248:GLU:CB	2.66	0.44
1:A:62:HIS:CD2	1:A:92:THR:OG1	2.72	0.43
1:B:258:GLY:O	1:B:259:ILE:CB	2.68	0.42
1:A:333:VAL:O	1:A:337:ARG:N	2.53	0.42
1:A:401:GLU:O	1:A:405:MET:SD	2.77	0.42
1:B:324:GLY:O	1:B:326:THR:N	2.52	0.41
1:B:218:GLN:O	1:B:299:ALA:N	2.53	0.41
1:B:333:VAL:O	1:B:337:ARG:N	2.53	0.41
1:A:224:GLY:O	1:A:225:THR:C	2.58	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	391/421 (93%)	354 (90%)	26 (7%)	11 (3%)	8	29
1	B	393/421 (93%)	358 (91%)	27 (7%)	8 (2%)	11	40

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	784/842 (93%)	712 (91%)	53 (7%)	19 (2%)	9	34

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	242	ALA
1	A	248	GLU
1	A	254	TYR
1	A	256	GLU
1	B	242	ALA
1	A	241	ILE
1	A	270	ALA
1	A	325	PRO
1	B	241	ILE
1	B	325	PRO
1	B	256	GLU
1	B	272	LYS
1	A	305	ILE
1	B	259	ILE
1	A	249	GLY
1	A	303	ASN
1	B	248	GLU
1	B	345	ILE
1	A	345	ILE

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	312/340 (92%)	303 (97%)	9 (3%)	55	88
1	B	314/340 (92%)	298 (95%)	16 (5%)	33	71
All	All	626/680 (92%)	601 (96%)	25 (4%)	42	80

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	LEU
1	A	132	LEU
1	A	202	SER
1	A	212	ASP
1	A	237	LYS
1	A	308	GLU
1	A	364	TYR
1	A	398	THR
1	A	401	GLU
1	B	8	LEU
1	B	89	LEU
1	B	132	LEU
1	B	163	LYS
1	B	195	VAL
1	B	212	ASP
1	B	250	ASN
1	B	256	GLU
1	B	260	ASP
1	B	264	LEU
1	B	308	GLU
1	B	364	TYR
1	B	381	MET
1	B	397	VAL
1	B	398	THR
1	B	401	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	SO4	A	1422	-	4,4,4	0.36	0	6,6,6	0.39	0
2	SO4	A	1423	-	4,4,4	0.46	0	6,6,6	0.48	0
2	SO4	B	1422	-	4,4,4	0.38	0	6,6,6	0.43	0
2	SO4	B	1423	-	4,4,4	0.44	0	6,6,6	0.24	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SO4	A	1422	-	-	0/0/0/0	0/0/0/0
2	SO4	A	1423	-	-	0/0/0/0	0/0/0/0
2	SO4	B	1422	-	-	0/0/0/0	0/0/0/0
2	SO4	B	1423	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	395/421 (93%)	-0.12	22 (5%) 24 30	37, 71, 128, 160	0
1	B	397/421 (94%)	0.03	24 (6%) 21 26	41, 76, 141, 228	0
All	All	792/842 (94%)	-0.04	46 (5%) 22 28	37, 74, 132, 228	0

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	308	GLU	4.9
1	A	270	ALA	4.4
1	B	326	THR	4.2
1	B	254	TYR	4.1
1	B	270	ALA	4.0
1	A	212	ASP	3.7
1	B	247	ASN	3.5
1	B	336	GLU	3.4
1	A	312	THR	3.4
1	B	246	ARG	3.4
1	B	332	LYS	3.4
1	A	271	ASN	3.3
1	A	250	ASN	3.3
1	B	212	ASP	3.3
1	A	247	ASN	3.2
1	A	395	TYR	3.2
1	A	209	LYS	3.1
1	B	211	GLU	3.0
1	B	5	LEU	2.9
1	B	294	ASP	2.9
1	B	314	ASN	2.8
1	A	314	ASN	2.7
1	A	255	ASN	2.7
1	B	252	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	256	GLU	2.7
1	A	249	GLY	2.6
1	B	312	THR	2.5
1	A	50	GLY	2.5
1	B	256	GLU	2.4
1	A	328	PRO	2.4
1	A	336	GLU	2.3
1	B	20	GLU	2.3
1	B	394	GLU	2.3
1	B	311	LYS	2.3
1	B	395	TYR	2.3
1	A	269	GLU	2.2
1	A	78	ASN	2.2
1	A	272	LYS	2.2
1	A	254	TYR	2.2
1	A	16	ARG	2.2
1	B	209	LYS	2.2
1	B	393	ASP	2.1
1	B	306	THR	2.1
1	A	396	ASN	2.1
1	B	257	ASN	2.1
1	A	119	ARG	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	SO4	A	1422	5/5	0.18	2.15	64,64,66,67	0
2	SO4	B	1422	5/5	0.25	1.93	61,65,66,67	0
2	SO4	A	1423	5/5	0.20	1.10	65,67,68,70	0
2	SO4	B	1423	5/5	0.17	0.32	63,67,68,68	0

6.5 Other polymers

There are no such residues in this entry.